



Quantum Monte Carlo calculations of lepton-nucleus interactions

FNAL Neutrino Seminar
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Saori Pastore
Washington University in St Louis

<https://physics.wustl.edu/quantum-monte-carlo-group>

Quantum Monte Carlo Group @ WashU
Lorenzo Andreoli (PD) Jason Bub (GS) Garrett King (GS) Maria Piarulli and Saori Pastore

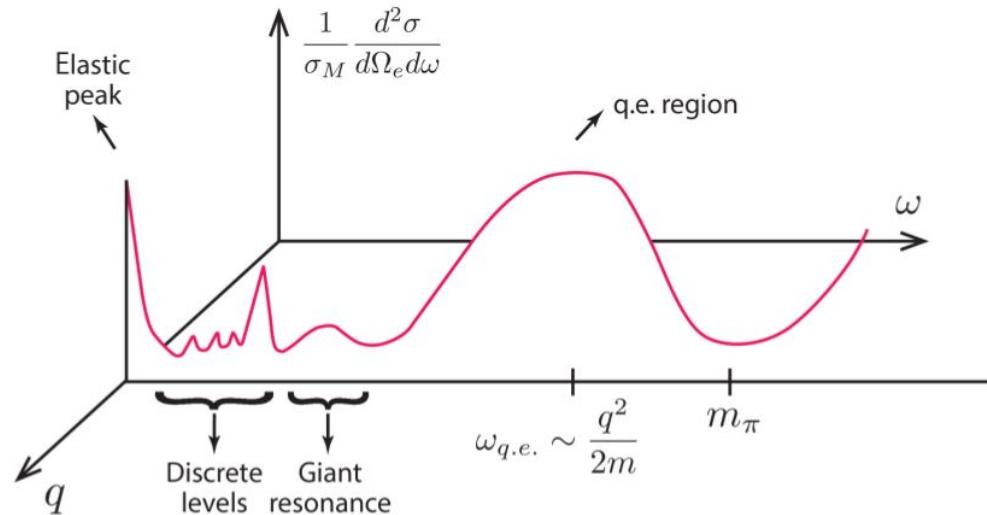
Computational Resources awarded by the DOE ALCC and INCITE programs

Nuclei for Fundamental Symmetries & Neutrinos

An accurate understanding of nuclear structure and dynamics in a wide range of energy and momentum transferred is required in order to disentangle new physics from nuclear effects.

In this talk, I will focus on the **role of many-body correlations and currents in selected nuclear electroweak observables** at different kinematics.

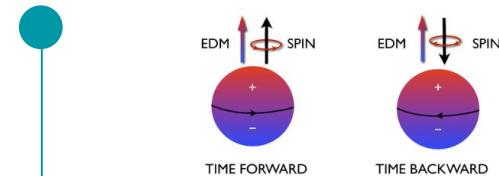
Electron-Nucleus Scattering Cross Section



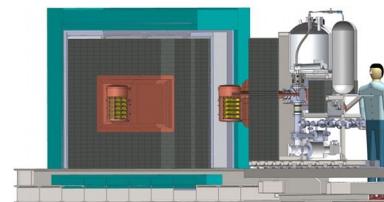
Energy and momentum transferred (ω, q)

Current and planned experimental programs rely on theoretical calculations at different kinematics

Ground States'
Electroweak Moments,
Form Factors, Radii



Neutrinoless Double
Beta Decay,
Muon-Capture



Accelerator Neutrino
Experiments,
Lepton-Nucleus XSecs

$(\omega, q) \sim 0$ MeV

$\omega \sim \text{few MeVs}$
 $q \sim 0$ MeV

$\omega \sim \text{few MeVs}$
 $q \sim 10^2$ MeV

$\omega \sim \text{tens of MeVs}$

$\omega \sim 10^2$ MeV



FRIB

Electromagnetic
Decay, Beta Decay,
Double Beta Decay &
inverse processes



Nuclear Rates for
Astrophysics



Strategy

Validate the Nuclear Model against available data for strong and electroweak observables

- Energy Spectra, Electromagnetic Form Factors, Electromagnetic Moments, ...
- Electromagnetic and Beta decay rates, ...
- Muon Capture Rates, ...
- Electron-Nucleus Scattering Cross Sections, ...

Use attained information to make (accurate) predictions for BSM searches and precision tests

- EDMs, Hadronic PV, ...
- BSM searches with beta decay, ...
- Neutrinoless double beta decay, ...
- Neutrino-Nucleus Scattering Cross Sections, ...
- ...

Microscopic (or *ab initio*) Description of Nuclei

Goal:

Comprehensive theory that describes quantitatively and predictably nuclear structure and reactions

Requirements:

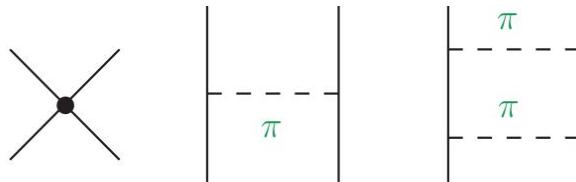
- Accurate understanding of the interactions/correlations between nucleons in pairs, triplets, ...
(two- and three-nucleon forces)
- Accurate understanding of the electroweak interactions of leptons with nucleons, correlated nucleon-pairs, ...
(one- and two-body electroweak currents)
- Computational methods to solve the many-body nuclear problem of strongly interacting particles

Many-body Nuclear Interactions

Many-body Nuclear Hamiltonian

$$H = T + V = \sum_{i=1}^A t_i + \sum_{i < j} v_{ij} + \sum_{i < j < k} V_{ijk} + \dots$$

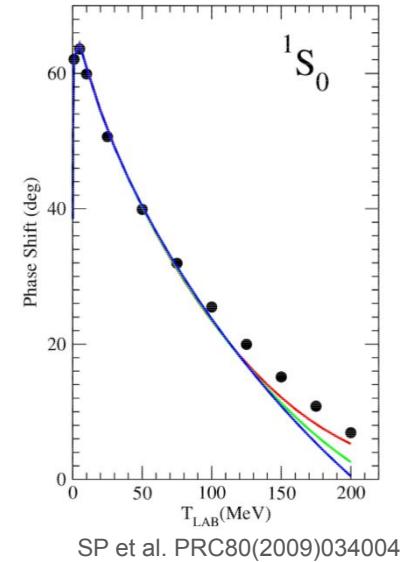
v_{ij} and V_{ijk} are two- and three-nucleon operators based on experimental data fitting; fitted parameters subsume underlying QCD dynamics



Contact term: short-range

Two-pion range: intermediate-range $r \propto (2 m_\pi)^{-1}$

One-pion range: long-range $r \propto m_\pi^{-1}$



In Quantum Monte Carlo methods we use:

AV18+UIX; AV18+IL7 Wiringa, Schiavilla, Pieper *et al.*

chiral πN N2LO+N2LO Gerzelis, Tews, Lynn *et al.*

chiral $\pi N\Delta$ N3LO+N2LO Piarulli *et al.* Norfolk Models

Quantum Monte Carlo Methods

Minimize the expectation value of the nuclear Hamiltonian: $H = T + \textcolor{blue}{v}_{ij} + \textcolor{red}{V}_{ijk}$

$$E_V = \frac{\langle \Psi_V | H | \Psi_V \rangle}{\langle \Psi_V | \Psi_V \rangle} \geq E_0$$

using the trial wave function:

$$|\Psi_V\rangle = \left[\mathcal{S} \prod_{i < j} \left(1 + \textcolor{blue}{U}_{ij} + \sum_{k \neq i, j} \textcolor{red}{U}_{ijk} \right) \right] \left[\prod_{i < j} f_c(r_{ij}) \right] |\Phi_A(JMTT_3)\rangle$$

Further improve the trial wave function by eliminating spurious contaminations via a Green's Function Monte Carlo (GFMC) propagation in imaginary time

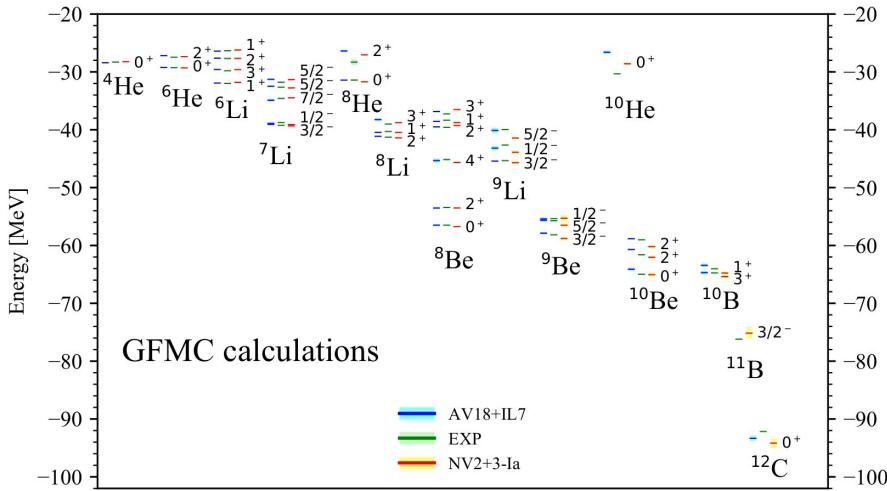
$$\begin{aligned} \Psi(\tau) &= \exp[-(H - E_0)\tau] \Psi_V = \sum \exp[-(E_n - E_0)\tau] a_n \psi_n \\ \Psi(\tau \rightarrow \infty) &= a_0 \psi_0 \end{aligned}$$

AV18+UIX; AV18+IL7 Wiringa, Schiavilla, Pieper *et al.*

chiral πN **N2LO+N2LO** Gerzelis, Tews, Lynn *et al.*

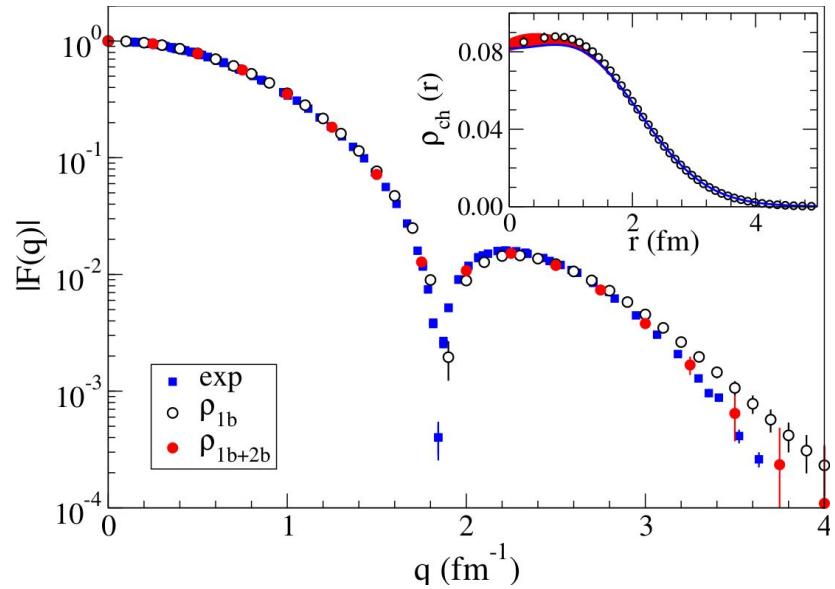
chiral $\pi N \Delta$ **N3LO+N2LO** Piarulli *et al.* **Norfolk Models**

Energies and Shapes of Nuclei

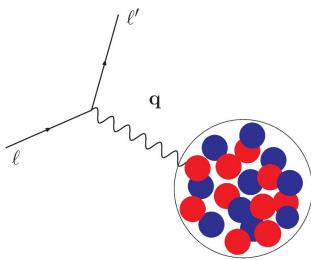


Spectra of light nuclei
Piarulli et al. PRL120(2018)052503

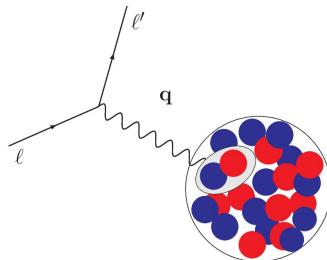
Charge form factor ^{12}C
Lovato et al. PRL111(2013)092501



Many-body Nuclear Electroweak Currents



one-body



two-body

- One-body currents: non-relativistic reduction of covariant nucleons' currents
- Two-body currents are a manifestation of two-nucleon correlations
- Electromagnetic two-body currents are required to satisfy current conservation

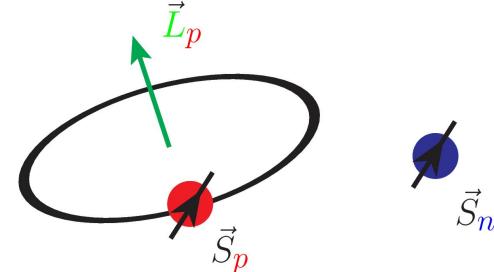
$$\mathbf{q} \cdot \mathbf{j} = [H, \rho] = [t_i + v_{ij} + V_{ijk}, \rho]$$

Nuclear Charge Operator

$$\rho = \sum_{i=1}^A \rho_i + \sum_{i < j} \rho_{ij} + \dots$$

Nuclear (Vector) Current Operator

$$\mathbf{j} = \sum_{i=1}^A \mathbf{j}_i + \sum_{i < j} \mathbf{j}_{ij} + \dots$$



Magnetic Moment: Single Particle Picture

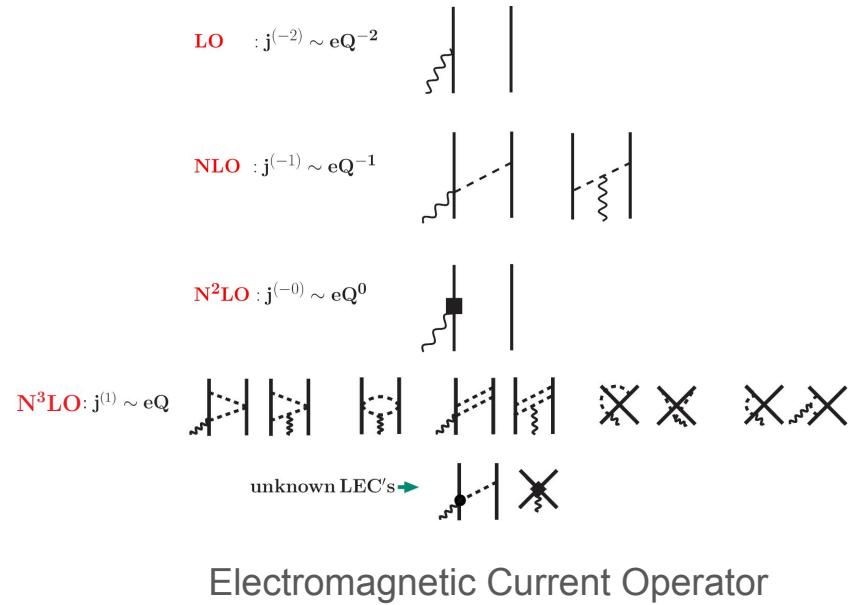
Many-body Currents: Available Models

- **Meson Exchange Currents (MEC)**

Constrain the MEC current operators by imposing that the current **conservation relation is satisfied with the given two-body potential**

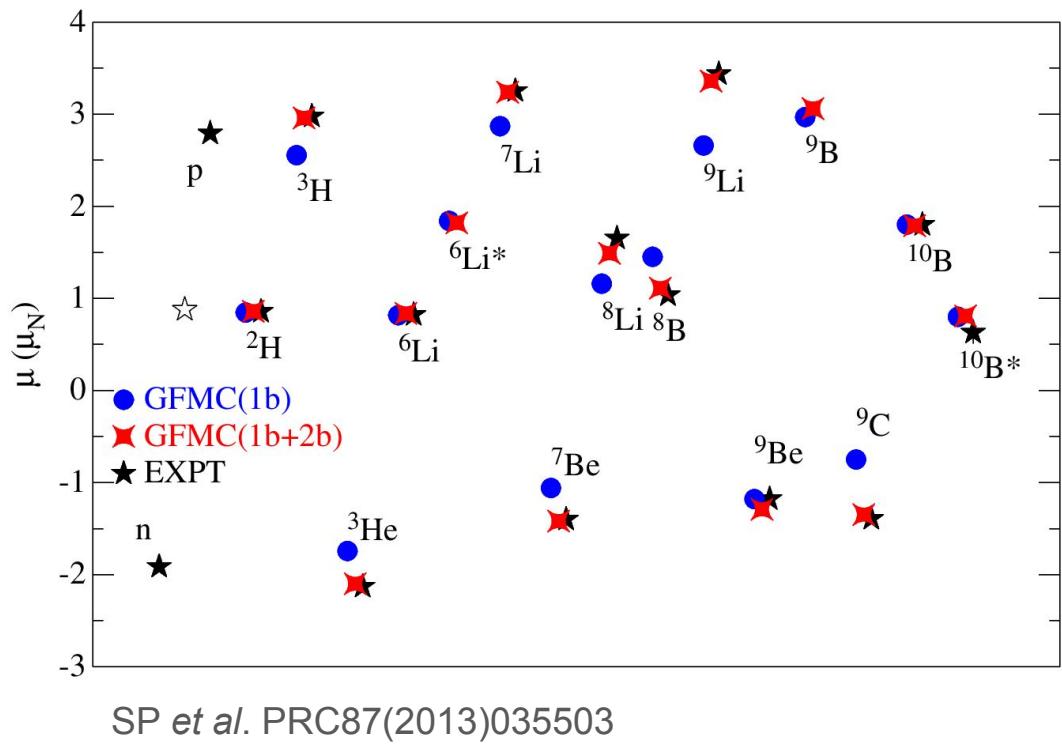
- **Chiral Effective Field Theory Currents**

Are constructed consistently with the two-body chiral potential; Unknown parameters, or Low Energy Constants (**LECs**), need to be **determined by either fits to experimental data or by QCD calculations, as well as nucleonic form factors**

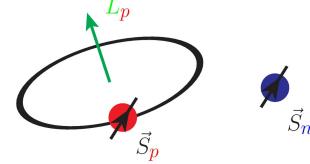


SP *et al.* PRC78(2008)064002, PRC80(2009)034004,
PRC84(2011)024001, PRC87(2013)014006
Park *et al.* NPA596(1996)515, Phillips (2005)
Kölling *et al.* PRC80(2009)045502 & PRC84(2011)054008

Magnetic Moments of Light Nuclei



Single particle picture



$$\mu_N(1b) = \sum_i [(L_i + g_p S_i)(1 + \tau_{i,z})/2 + g_n S_i(1 - \tau_{i,z})/2]$$

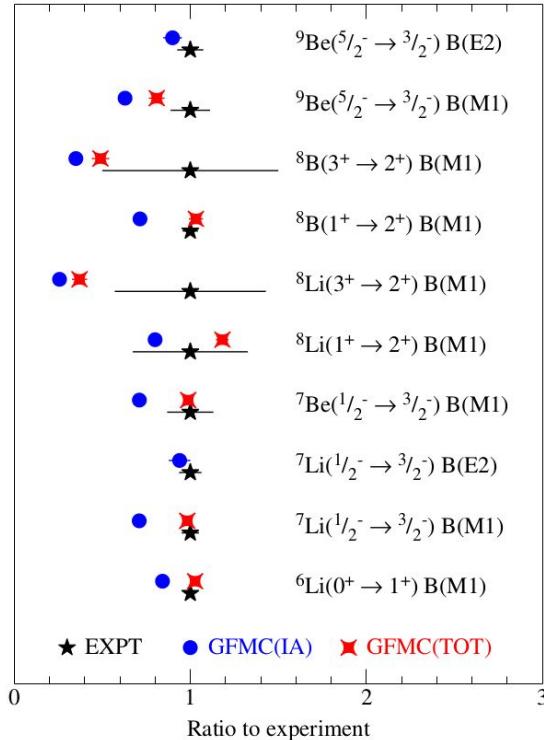
Small two-body current effects



Large two-body current effects



Electromagnetic Transitions in Low-lying States



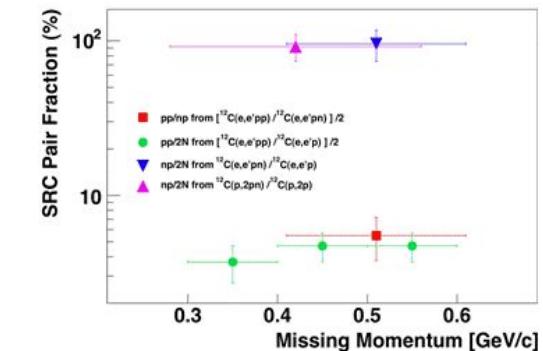
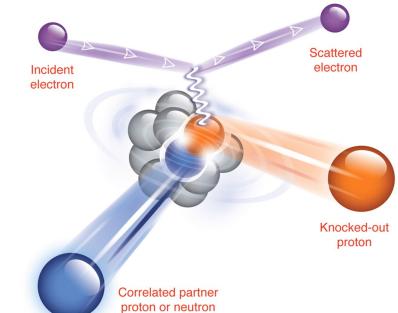
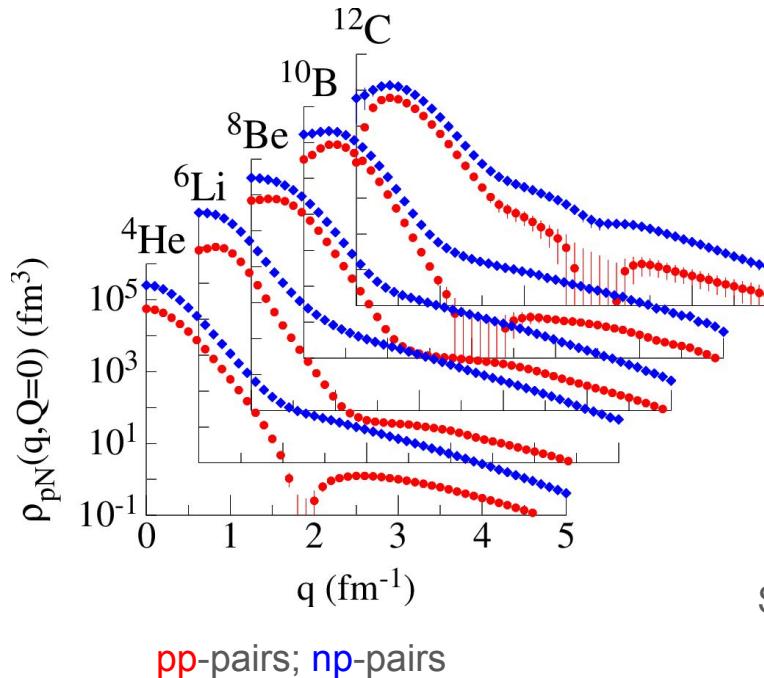
- Two-body electromagnetic currents bring the theory in a better agreement with the experimental data
- Significant corrections found in ${}^9\text{Be}$ and ${}^9\text{C}$'s magnetic moments where two-body currents provide a $\sim 40\%$ contribution
- In electromagnetic transitions in low-lying nuclear states, two-body currents are at the 10-20% level

Electron-Nucleus Scattering



Nuclear properties are strongly affected by two-body correlations and currents in a wide range of energy and momentum transfer

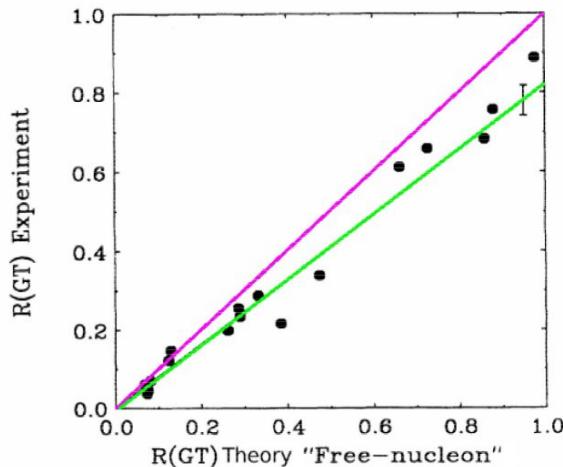
Two-body momentum distribution
Wiringa et al. PRC89(2014)024305



Subedi et al. Science320(2008)1475

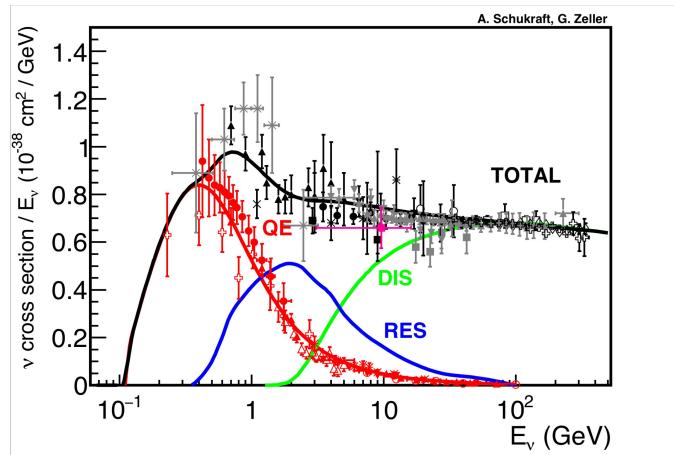
Neutrino-Nucleus Interactions

Low energy and momentum:
Beta Decay Matrix Elements



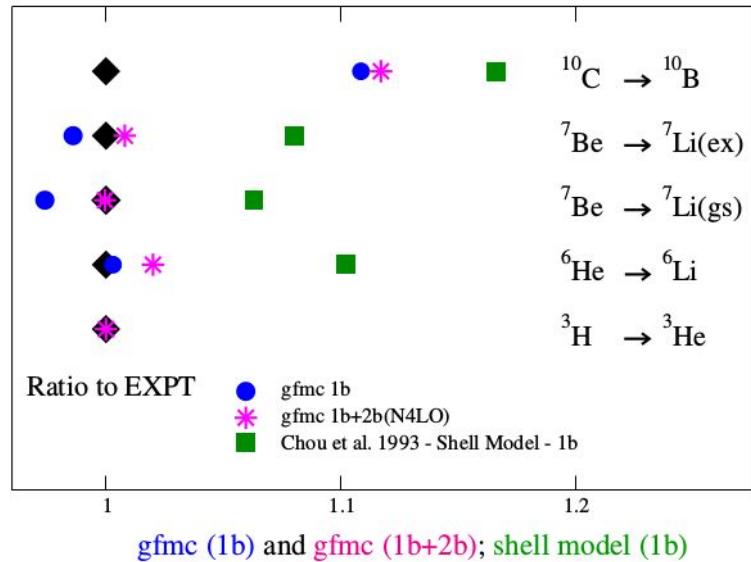
Chou et al. PRC47(1993)163

High Energy (on Nuclear Physics Scale):
Neutrino-Nucleus Cross Section

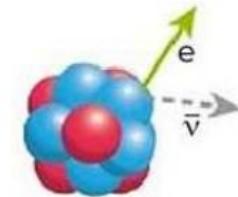


Formaggio and Zeller

Beta decay in light nuclei correlations

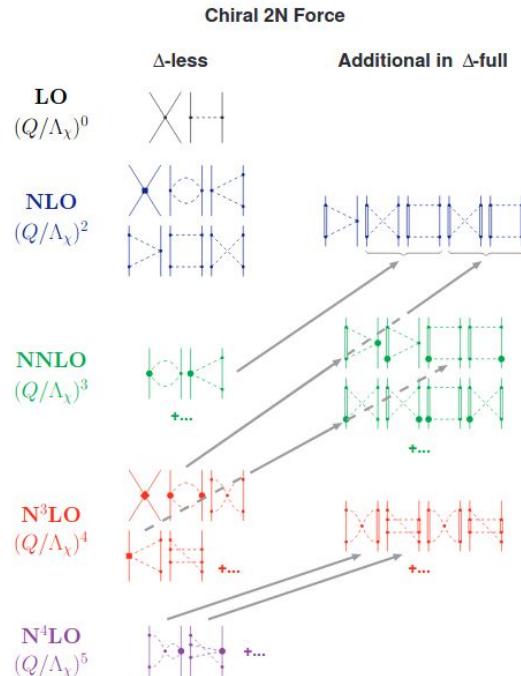


$$(\textcolor{red}{Z}, \textcolor{blue}{N}) \rightarrow (\textcolor{red}{Z+1}, \textcolor{blue}{N-1}) + \textcolor{green}{e} + \bar{\nu}_e$$



SP *et al.* PRC97(2018)022501

Norfolk Two- and Three-body Potentials

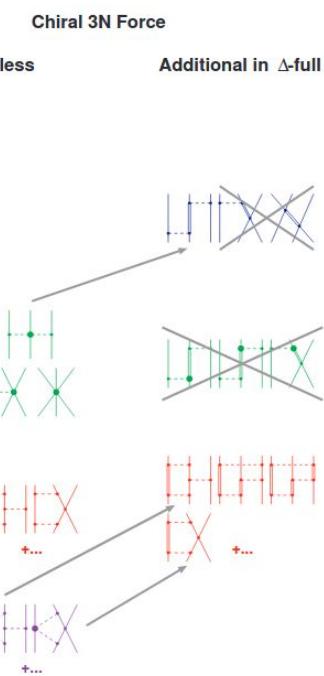


Norfolk Chiral Potentials

NV2+3

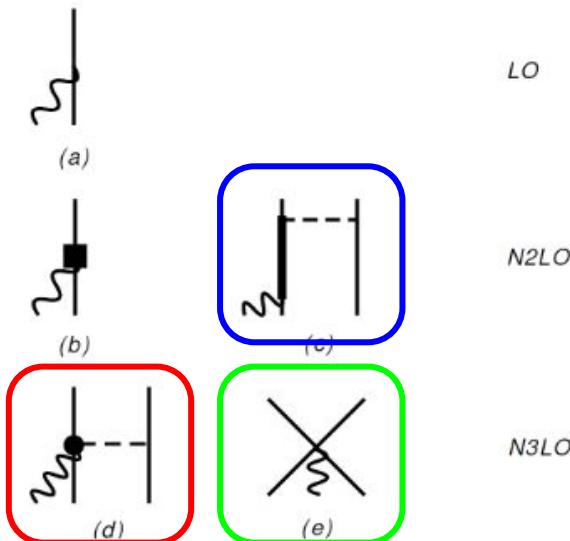
developed in Piarulli *et al.*
PRC91(2015)024003
PRC94(2016)054007

26 LECs fitted to np and pp
Granada database
(2600-3600 data points) with
a chi-square/datum ~1



Figs. credit Entem and Machleidt Phys.Rept.503(2011)1

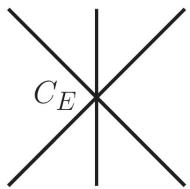
Axial currents



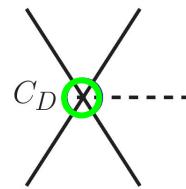
Two body currents of one pion range
(red and blue) do not involve
additional LECs

Contact current involves the LEC c_D

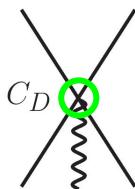
Three-body Force and the Axial Contact Current



Three-body force



Axial two-body contact current

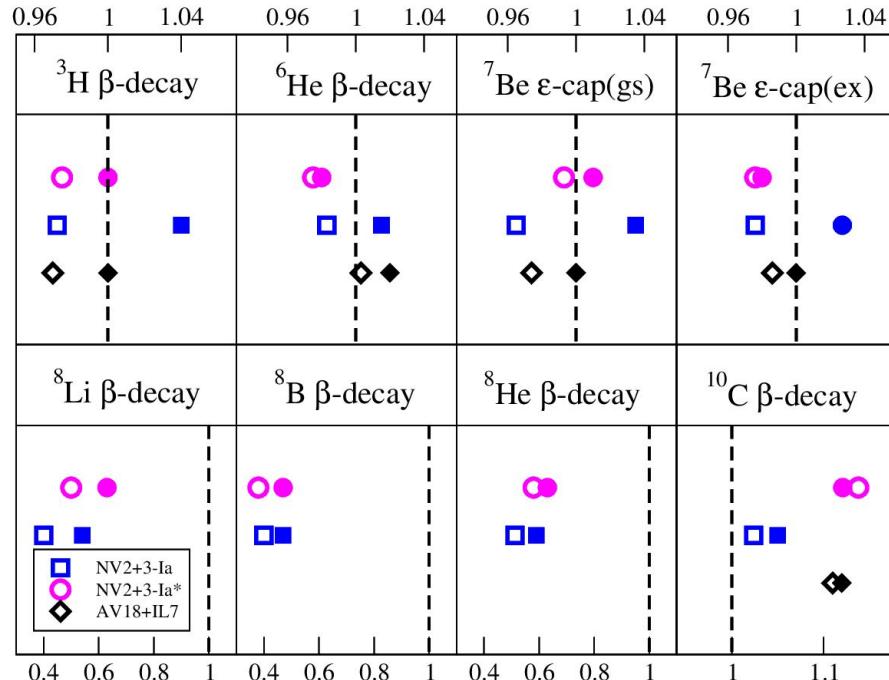


LECs c_D and c_E are fitted to:

- trinucleon B.E. and nd doublet scattering length in **NV2+3-1a**
- trinucleon B.E. and Gamow-Teller matrix element of tritium **NV2+3-1a***

Baroni *et al.* PRC98(2018)044003

Beta Decay and Electron Capture in Light Nuclei



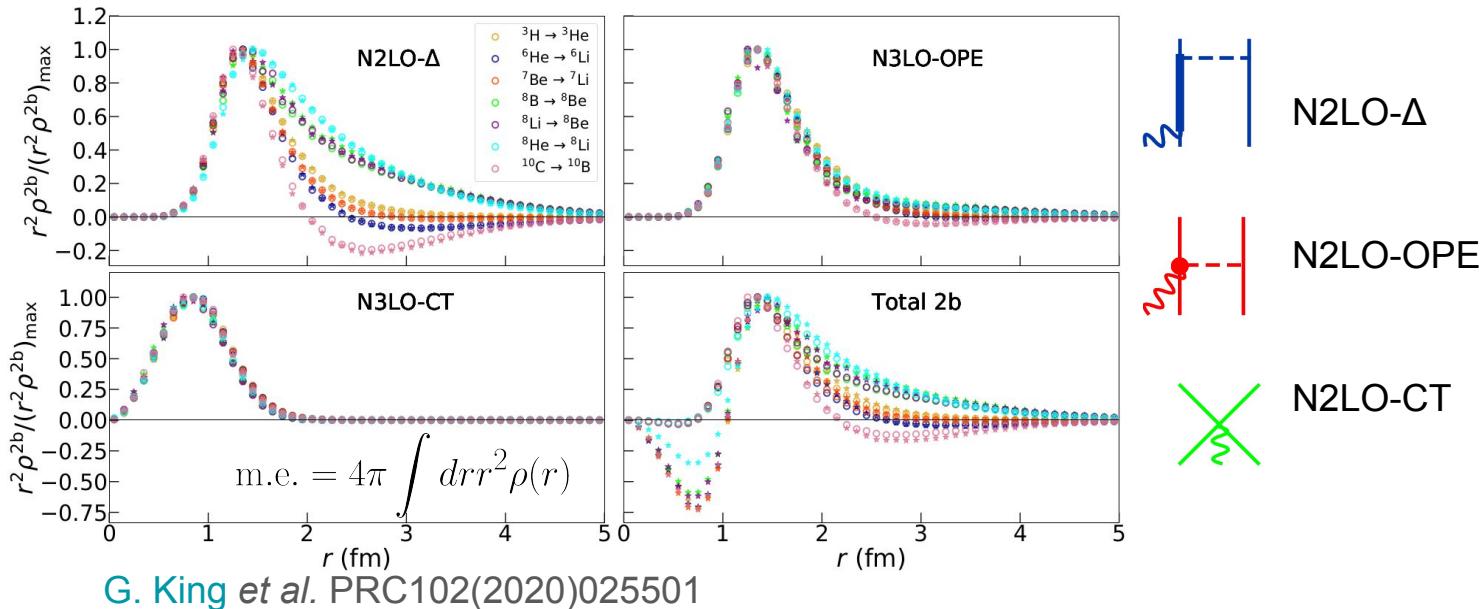
G. King *et al.* PRC102(2020)025501

Calculations based on

- chiral interactions and currents
NV2+3-Ia Norfolk unstarred
NV2+3-Ia* Norfolk* starred
Piarulli *et al.* PRL120(2018)052503
Baroni *et al.* PRC98(2018)044003
- phenomenological **AV18+IL7**
potential and chiral axial currents
(hybrid calculation)

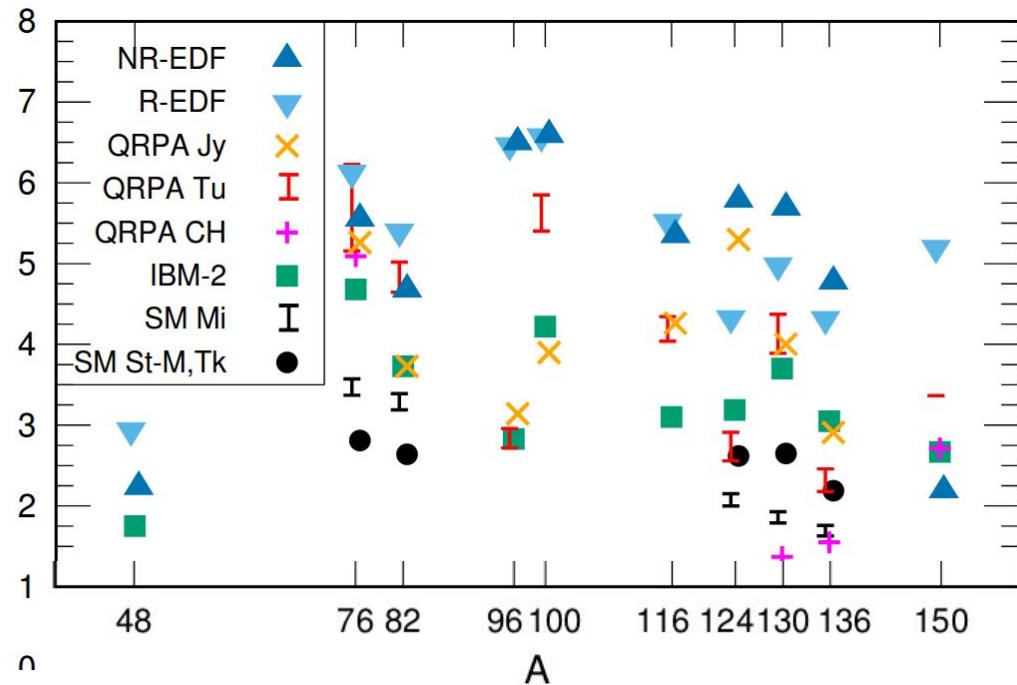
Two-body currents are small/negligible;
Results for $A=6-7$ are within 2% of data;
Results for $A=8$ are off by a 30-40%;
Results for $A=10$ are affected by the
second $J^\pi=(1^+)$ state in ^{10}B

Scaling and Universality of Short-Range Dynamics

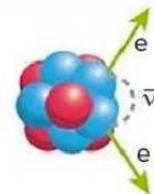
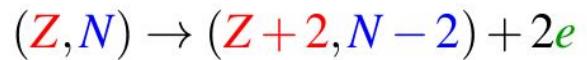


NV2+3-la empty circles; NV2+3-la* stars
Different colors refer to different transitions

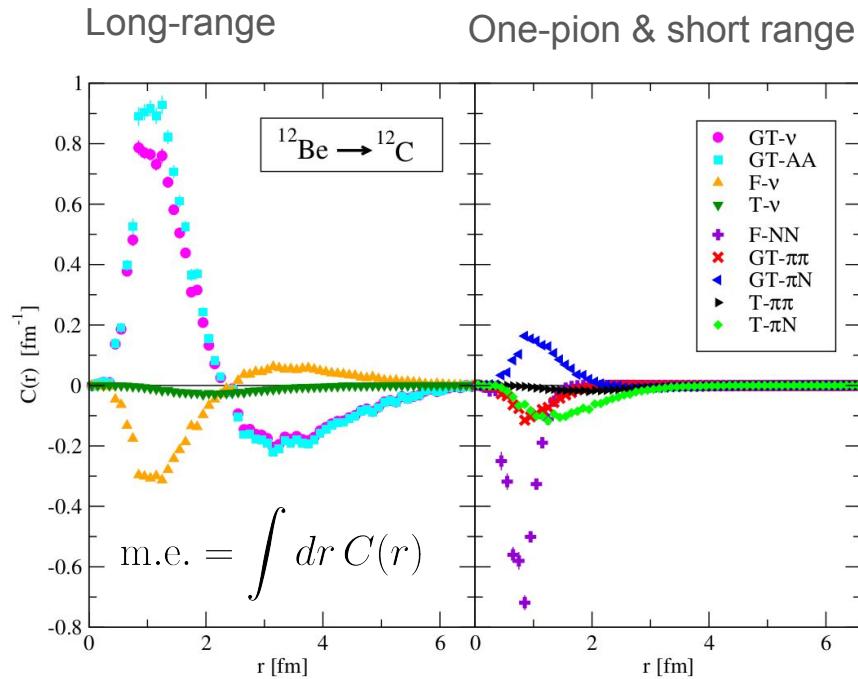
Neutrinoless Double Beta Decay



$$[T_{1/2}^{0\nu}]^{-1} = G_{0\nu}(Q, Z) |M_{0\nu}|^2 m_{\beta\beta}^2$$



Neutrinoless Double Beta Decay Matrix Elements



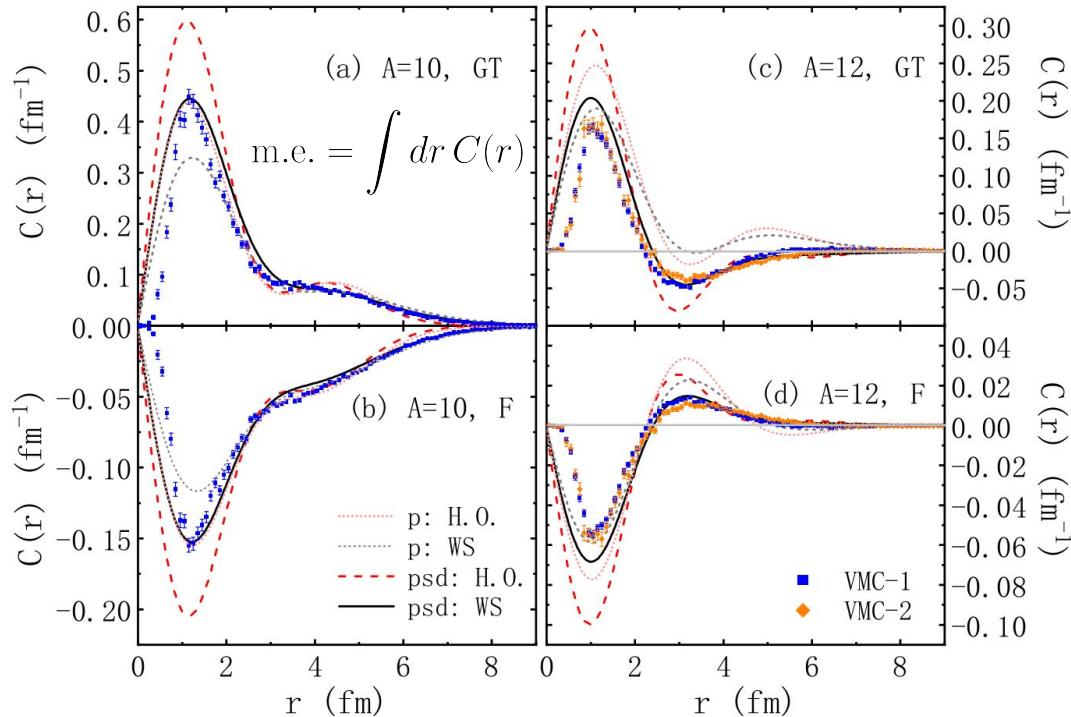
SP et al. PRC97(2018)014606



Cirigliano Dekens DeVries Graesser Mereghetti et al.
PLB769(2017)460, JHEP12(2017)082, PRC97(2018)065501

- Leading operators in neutrinoless double beta decay are two-body operators
- These observables are particularly sensitive to short-range and two-body physics
- Transition densities calculated in momentum space indicate that the momentum transfer in this process is of the order of ~ 200 MeV

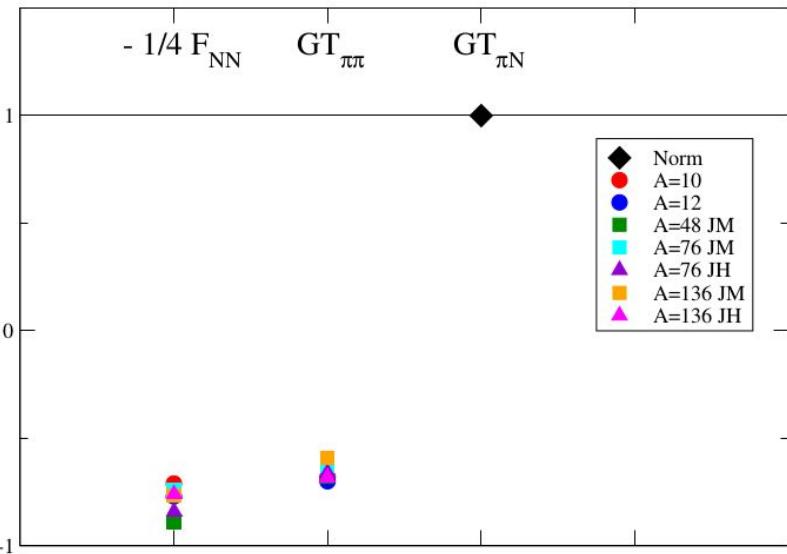
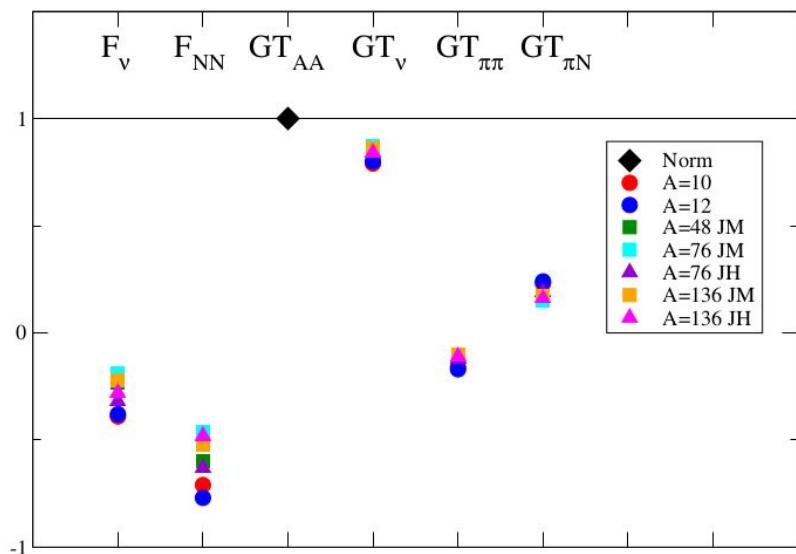
Comparison with Shell-Model Calculations



Closer agreement between Shell-Model calculations with Variational Monte Carlo results is reached by

- Increasing the size of the model space
- Wood-Saxon single particle wave functions are superior in describing the tails of the densities wrt harmonic oscillator wave functions
- Phenomenological Short-Range-Correlations functions further improve the agreement

Scaling up



JM = Javier Menendez private communication

JH = Hyvärinen et al. PRC91(2015)024613

Lepton-Nucleus scattering: Inclusive Processes

Electromagnetic Nuclear Response Functions

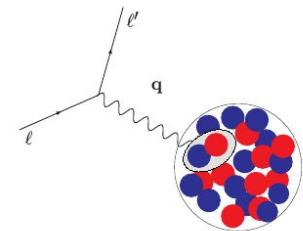
$$R_{\alpha}(q, \omega) = \sum_f \delta(\omega + E_0 - E_f) |\langle f | O_{\alpha}(\mathbf{q}) | 0 \rangle|^2$$

Longitudinal response induced by the charge operator $O_L = \rho$

Transverse response induced by the current operator $O_T = j$

5 Responses in neutrino-nucleus scattering

$$\frac{d^2 \sigma}{d\omega d\Omega} = \sigma_M [v_L R_L(\mathbf{q}, \omega) + v_T R_T(\mathbf{q}, \omega)]$$



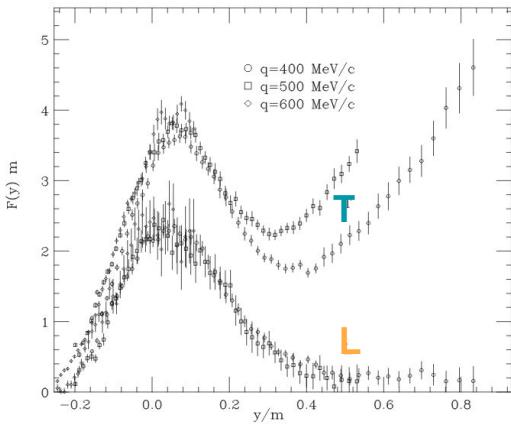
For a recent review see [Rocco Front.inPhys.8 \(2020\)116](#)

Lepton-Nucleus scattering: Data

Transverse Sum Rule

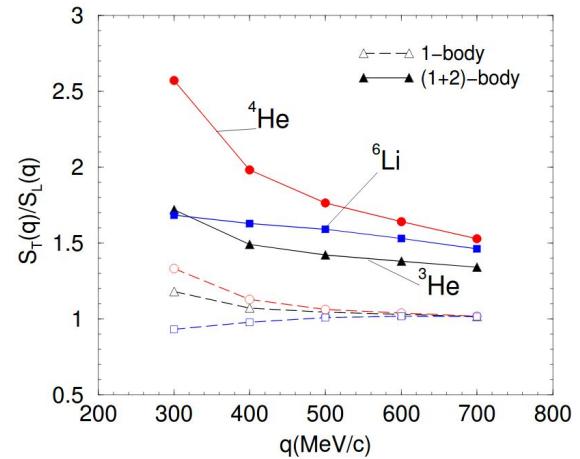
$$S_T(q) \propto \langle 0 | j^\dagger j | 0 \rangle \propto \langle 0 | j_{1b}^\dagger j_{1b} | 0 \rangle + \langle 0 | j_{1b}^\dagger j_{2b} | 0 \rangle + \dots$$

Observed transverse enhancement explained by the combined effect of two-body correlations and currents in the interference term



^{12}C Electromagnetic Data
Benhar et al. RMP80(2008)198

- $\langle j_{1b}^\dagger j_{1b} \rangle > 0$
Leading one-body term
- $\langle j_{1b}^\dagger j_{2b} v_\pi \rangle \propto \langle v_\pi^2 \rangle > 0$
Interference term

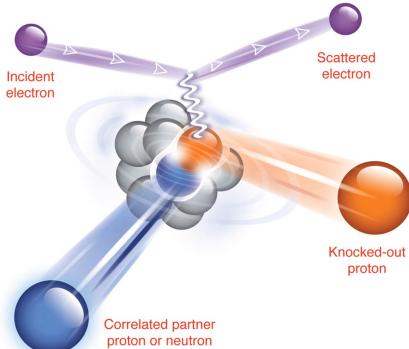


Transverse/Longitudinal Sum Rule
Carlson et al. PRC65(2002)024002

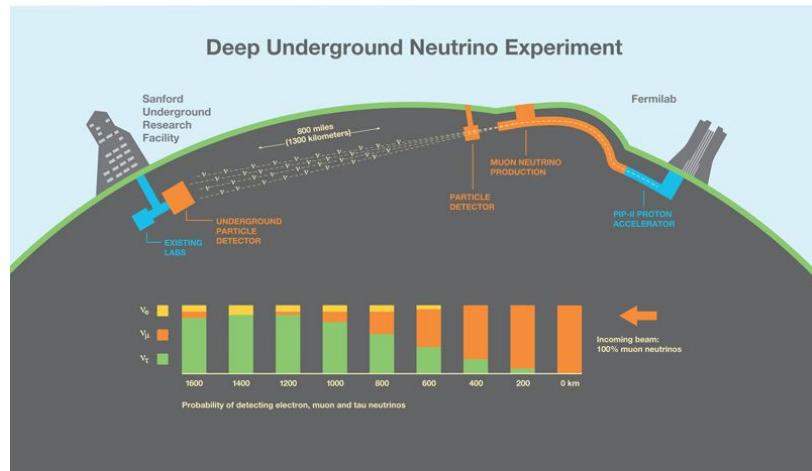
Beyond Inclusive: Short-Time-Approximation

Short-Time-Approximation Goals:

- Describe electroweak scattering from $A > 12$ without losing two-body physics
- Account for exclusive processes
- Incorporate relativistic effects



Subedi et al. Science 320(2008)1475



[Stanford Lab article](#)

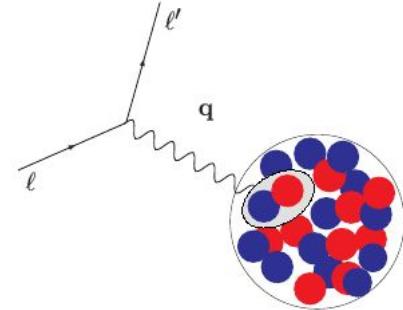
[e4u collaboration](#)

e4u

Short-Time-Approximation

Short-Time-Approximation:

- Based on Factorization
- Ratain two-body physics
- Correctly accounts for interference



$$R(q, \omega) = \int_{-\infty}^{\infty} \frac{dt}{2\pi} e^{i(\omega + E_0)t} \langle 0 | O^\dagger e^{-iHt} O | 0 \rangle$$

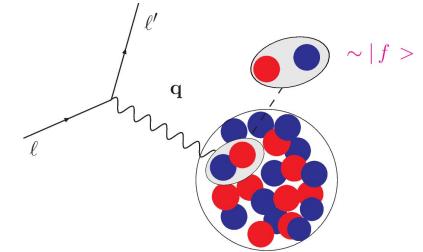
$$O_i^\dagger e^{-iHt} O_i + O_i^\dagger e^{-iHt} O_j + O_i^\dagger e^{-iHt} O_{ij} + O_{ij}^\dagger e^{-iHt} O_{ij}$$

$$H \sim \sum_i t_i + \sum_{i < j} v_{ij}$$

Short-Time-Approximation

Short-Time-Approximation:

- Response functions are given by the scattering from pairs of fully interacting nucleons that propagate into a correlated pair of nucleons
- Allows to retain both two-body correlations and currents at the vertex
- Provides “more” exclusive information in terms of nucleon-pair kinematics via the Response Densities



Response Functions

$$R_{\alpha}(q, \omega) = \sum_f \delta(\omega + E_0 - E_f) |\langle f | O_{\alpha}(\mathbf{q}) | 0 \rangle|^2$$

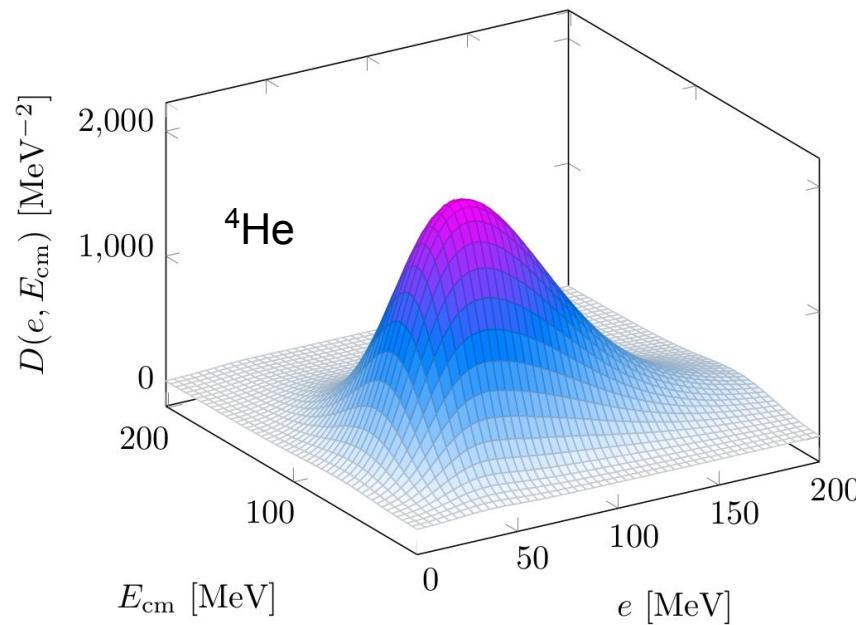
Response Densities

$$R(q, \omega) \sim \int \delta(\omega + E_0 - E_f) dP' dp' \mathcal{D}(p', P'; q)$$

P' and p' are the CM and relative momenta of the struck nucleon pair

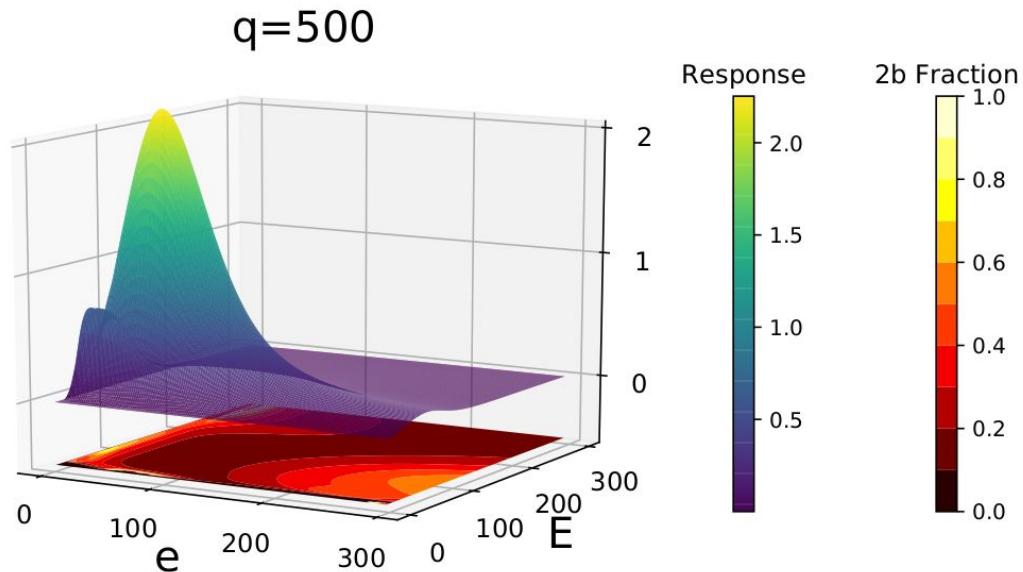
Transverse Response Density: e - ${}^4\text{He}$ scattering

Transverse Density $q = 500 \text{ MeV}/c$

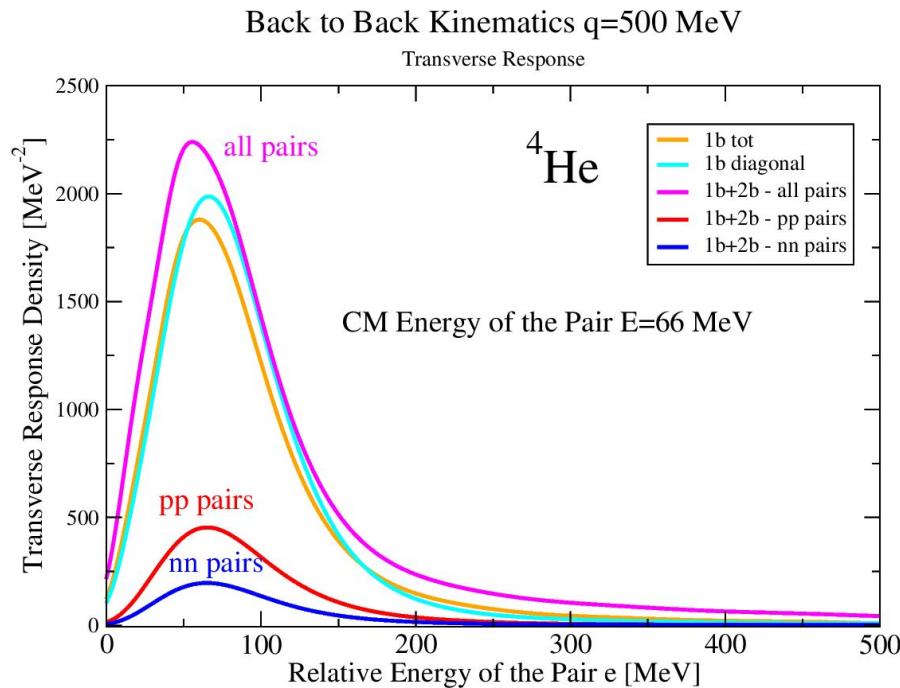


SP *et al.* PRC101(2020)044612

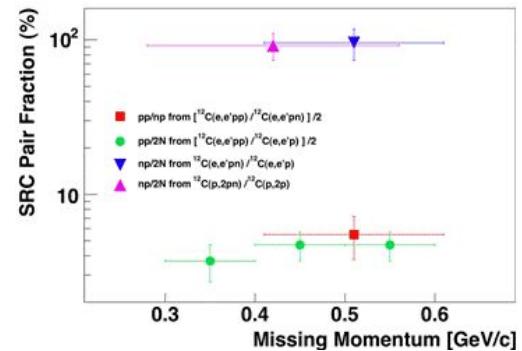
Transverse Response Density: two-body physics



e^- - 4He scattering in the back-to-back kinematic

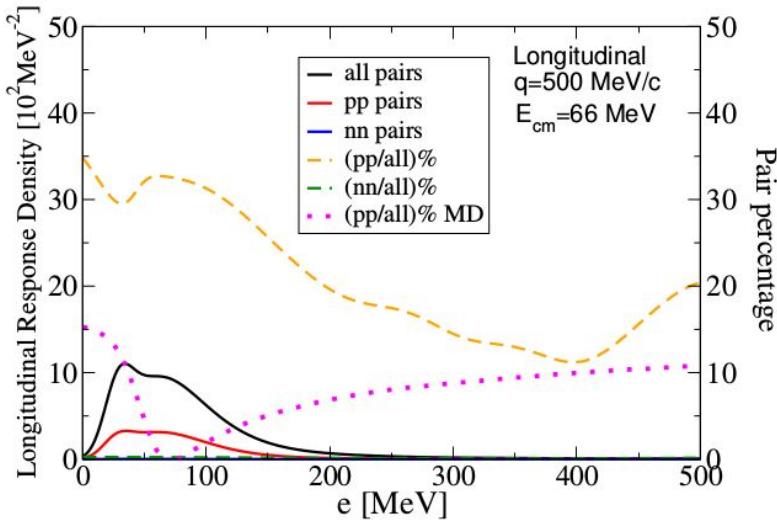


- pp pairs
- nn pairs
- all pairs 1body
- all pairs tot

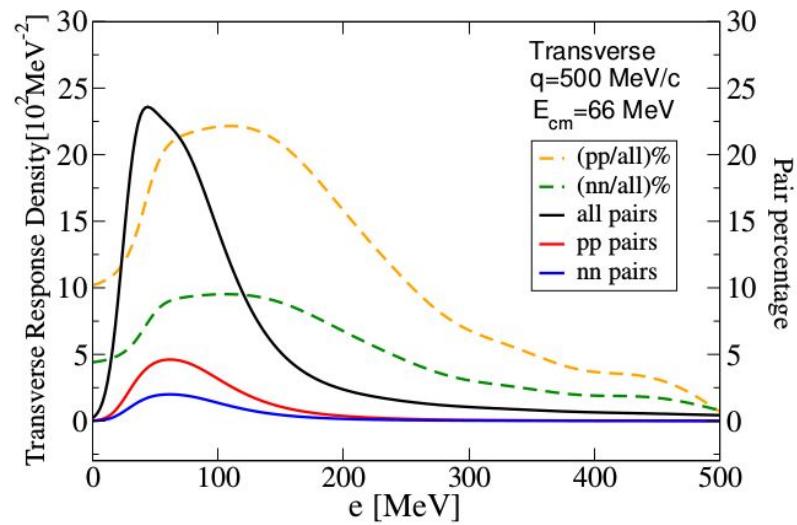


Subedi et al. Science 320(2008)1475

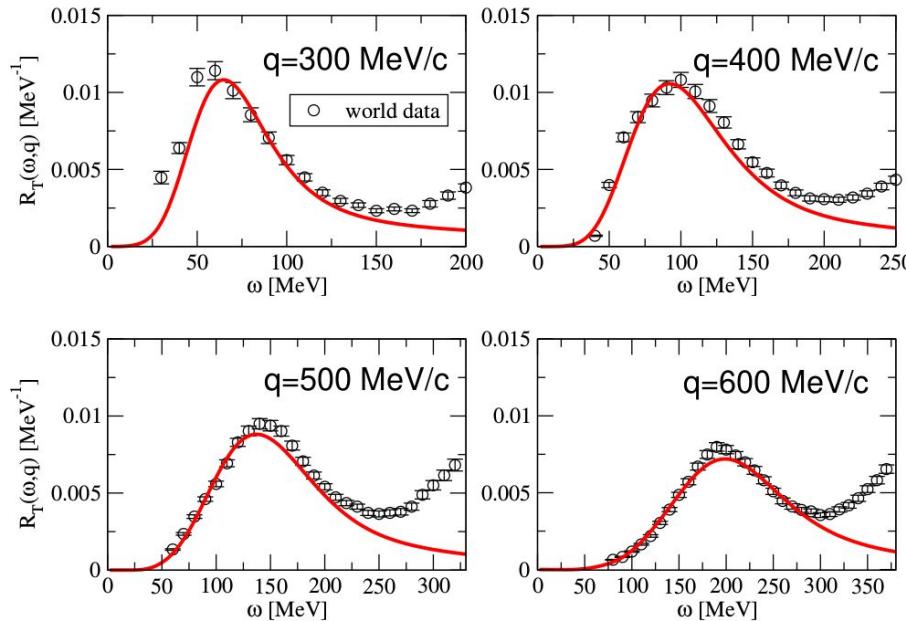
Back to back scattering and particle identity



tot
pp nn
pp/all % pp/all % from momentum distributions
nn/all %



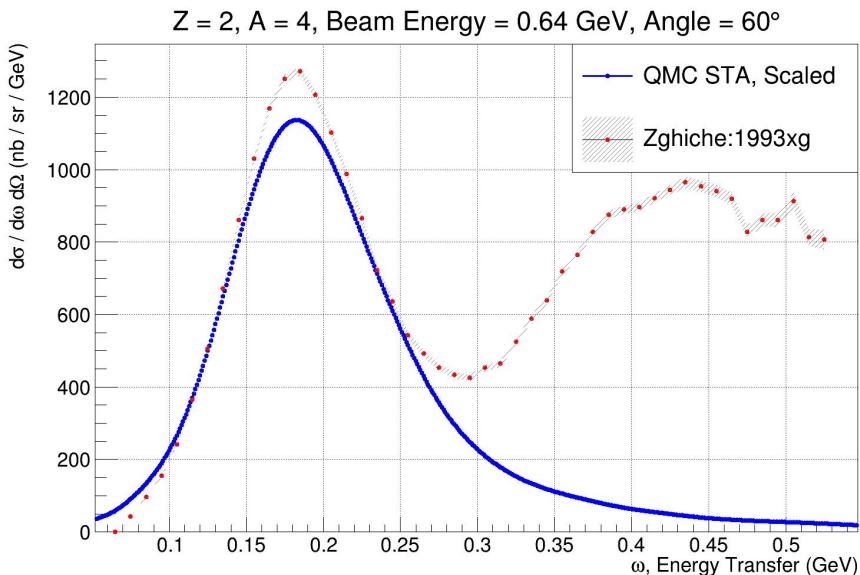
Helium-4 comparison with the data



SP *et al.* PRC101(2020)044612

Implementations in GENIE

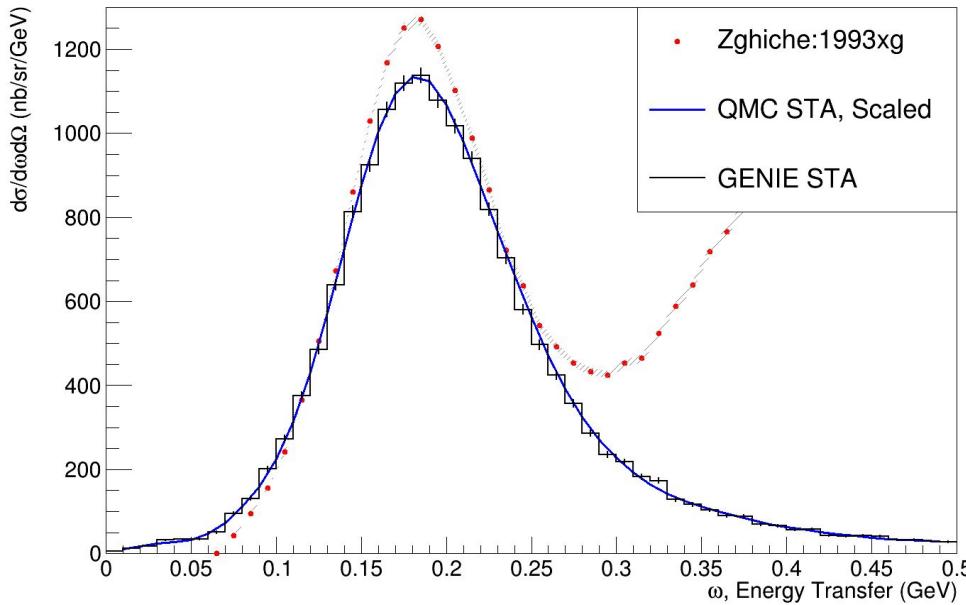
- STA responses used to build the cross sections
- Responses calculated on a finer grid of momentum transfer using scaling functions
- A finer grid in momentum transfer is required to achieve smoother interpolations



Barrow, Gardiner, Betancourt *et al.* PRD (2021)

GENIE validation using e-scattering

Z = 2, A = 4, Beam Energy = 0.64 GeV, Angle = $60^\circ \pm 0.25^\circ$

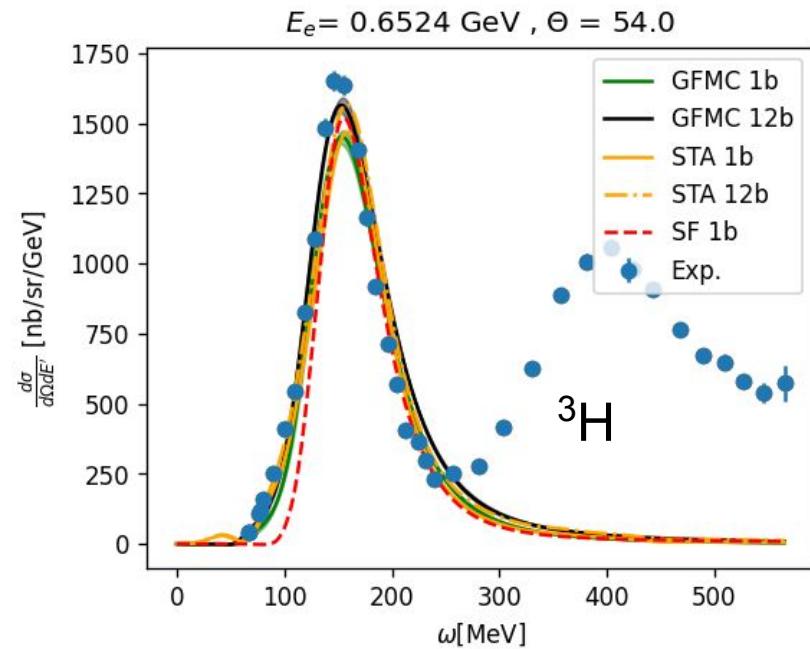
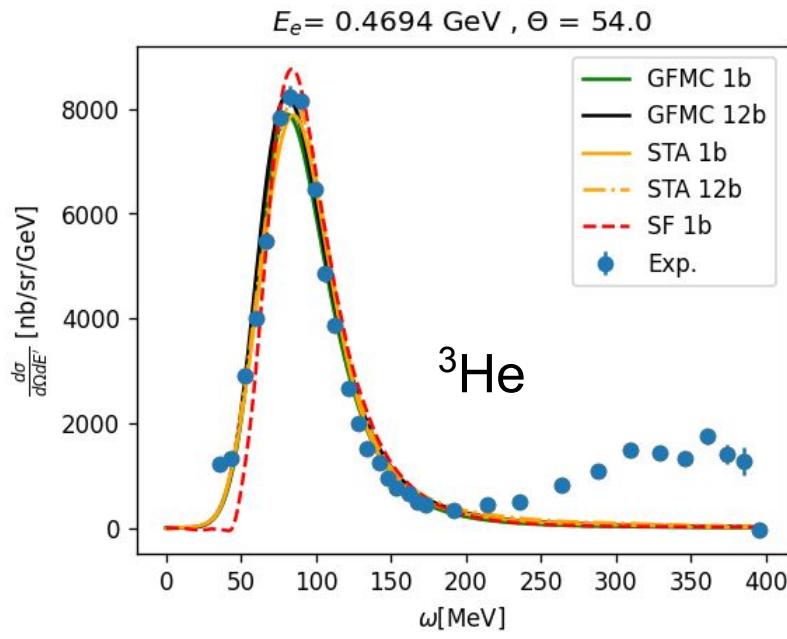


Ongoing work

- Implementation of moment-morphin interpolation techniques
- Implementations of response **Densities** in GENIE
- ^{12}C response densities with [Lorenzo Andreoli](#)

Barrow, Gardiner *et al.* to appear on PRD (2021)

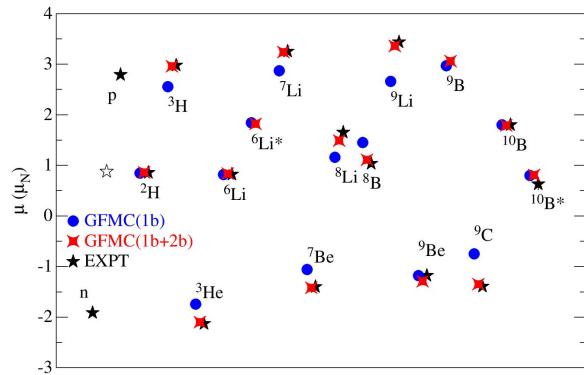
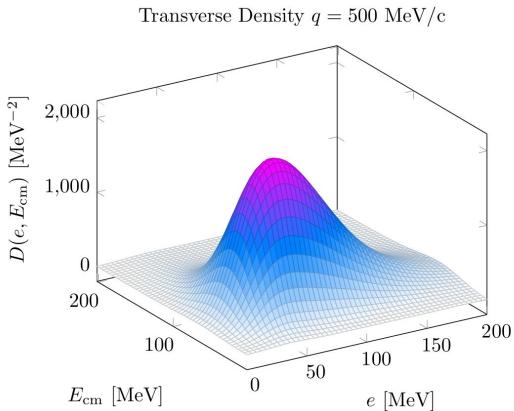
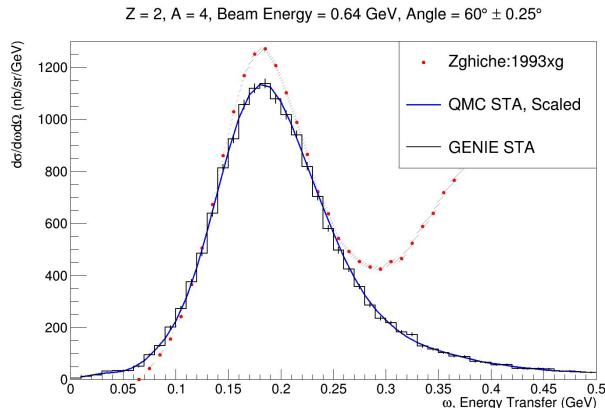
GFMC SF STA: Benchmark & error estimate



Rocco, Lovato, SP *et al.* ongoing

Summary and Outlook

Ab initio calculations of light nuclei yield a picture of nuclear structure and dynamics where **many-body effects play an essential role to explain available data.**



Close collaborations between
NP, LQCD, Pheno, Hep,
Comp, Expt, ...
are required to progress

It's a very exciting time!

Collaborators

WashU: Andreoli Bub King Piarulli

LANL: Baroni Carlson Cirigliano Gandolfi Hayes Mereghetti

JLab+ODU: Schiavilla

ANL: Lovato Rocco Wiringa

UCSD/UW: Dekens

Pisa U/INFN: Kievsky Marcucci Viviani

Salento U: Girlanda

Huzhou U: Dong Wang



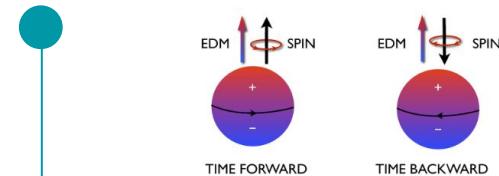
Theory Alliance
FACILITY FOR RARE ISOTOPE BEAMS



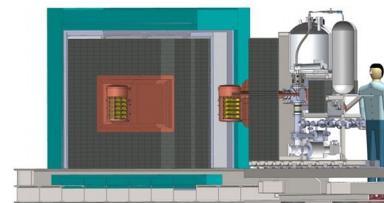
Office of
Science



Ground States'
Electroweak Moments,
Form Factors, Radii



Neutrinoless Double
Beta Decay,
Muon-Capture



Accelerator Neutrino
Experiments,
Lepton-Nucleus XSecs

$(\omega, q) \sim 0$ MeV

$\omega \sim \text{few MeVs}$
 $q \sim 0$ MeV

$\omega \sim \text{few MeVs}$
 $q \sim 10^2$ MeV

$\omega \sim \text{tens of MeVs}$

$\omega \sim 10^2$ MeV



FRIB

Electromagnetic
Decay, Beta Decay,
Double Beta Decay &
inverse processes



Nuclear Rates for
Astrophysics

